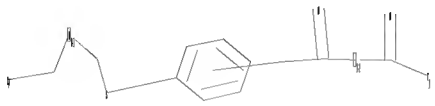
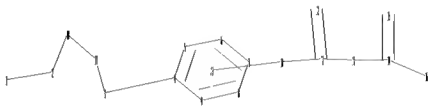
=>
Uploading C:\Program Files\Stnexp\Queries\rkc302.str





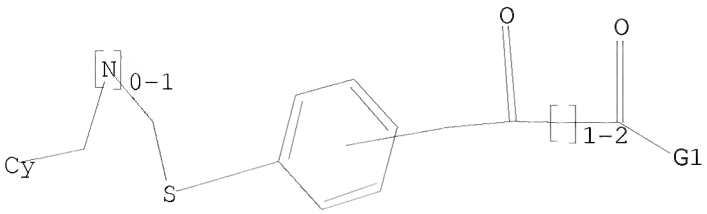
chain nodes :
1 2 3 10 11 12 13 14 15 16 17 18
ring nodes :
4 5 6 7 8 9
chain bonds :
1-2 2-18 3-4 3-17 10-11 11-12 11-13 13-14 14-15 14-16 17-18
ring bonds :
4-5 4-9 5-6 6-7 7-8 8-9
exact/norm bonds :
1-2 2-18 3-4 3-17 11-12 14-15 14-16 17-18
exact bonds :
10-11 11-13 13-14
normalized bonds :
4-5 4-9 5-6 6-7 7-8 8-9
isolated ring systems :
containing 4 :

G1:O,N

Match level :
1:Atom 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
21:Atom
Generic attributes :
1:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,N

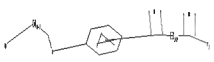
Structure attributes must be viewed using STN Express query preparation.

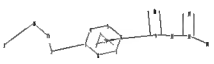
=> s l1 ful
FULL SEARCH INITIATED 12:07:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 13120 TO ITERATE

100.0% PROCESSED 13120 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\rkc302b.str





chain nodes :
1 2 9 10 11 12 13 14 15 16
ring nodes :
3 4 5 6 7 8
chain bonds :
1-16 2-3 2-15 9-11 9-10 11-12 12-13 12-14 15-16
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8
exact/norm bonds :
1-16 2-3 2-15 9-10 12-13 12-14 15-16
exact bonds :
9-11 11-12
normalized bonds :
3-4 3-8 4-5 5-6 6-7 7-8
isolated ring systems :

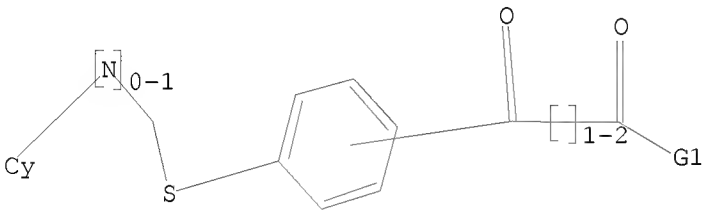
containing 3 :

G1:O,N

Match level :
1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 23:CLASS
Generic attributes :
1:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l3 ful
FULL SEARCH INITIATED 12:11:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 52566 TO ITERATE

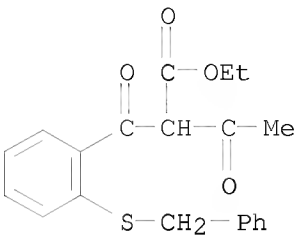
100.0% PROCESSED 52566 ITERATIONS 19 ANSWERS
SEARCH TIME: 00.00.01

L4 19 SEA SSS FUL L3

=> d 1-19

L4 ANSWER 1 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 857559-32-1 REGISTRY
ED Entered STN: 29 Jul 2005
CN Benzenepropanoic acid, α-acetyl-β-oxo-2-[(phenylmethyl)thio]-,
ethyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:

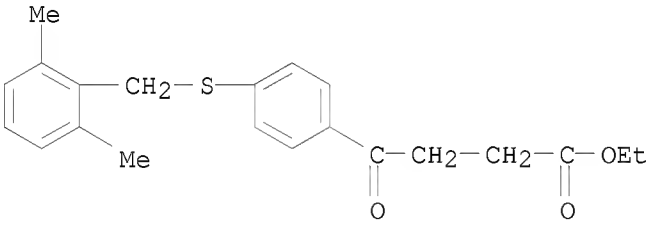
CN Acetoacetic acid, 2-[o-(benzylthio)benzoyl]-, ethyl ester (5CI)
MF C20 H20 O4 S
SR CAS EARLY REGISTRATIONS
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 2 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 847142-02-3 REGISTRY
ED Entered STN: 24 Mar 2005
CN Benzenebutanoic acid, 4-[[(2,6-dimethylphenyl)methyl]thio]-γ-oxo-, ethyl ester (CA INDEX NAME)
MF C21 H24 O3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

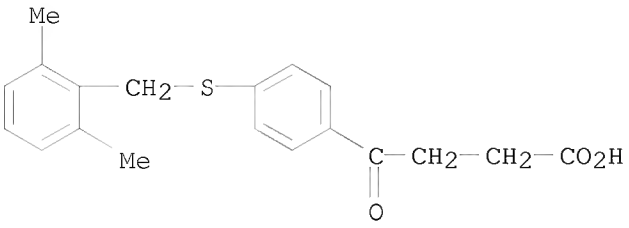


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 3 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 847142-00-1 REGISTRY
ED Entered STN: 24 Mar 2005
CN Benzenebutanoic acid, 4-[[(2,6-dimethylphenyl)methyl]thio]-γ-oxo- (CA INDEX NAME)
MF C19 H20 O3 S

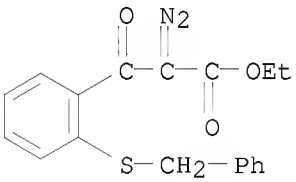
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

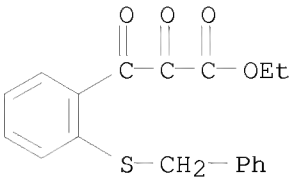
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 4 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 131327-55-4 REGISTRY
ED Entered STN: 11 Jan 1991
CN Benzenepropanoic acid, α-diazo-β-oxo-2-[(phenylmethyl)thio]-, ethyl ester (CA INDEX NAME)
MF C18 H16 N2 O3 S
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

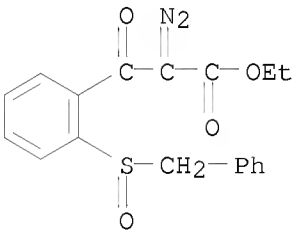
L4 ANSWER 5 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 120571-37-1 REGISTRY
ED Entered STN: 12 May 1989
CN Benzenepropanoic acid, α,β-dioxo-2-[(phenylmethyl)thio]-, ethyl ester (CA INDEX NAME)
MF C18 H16 O4 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

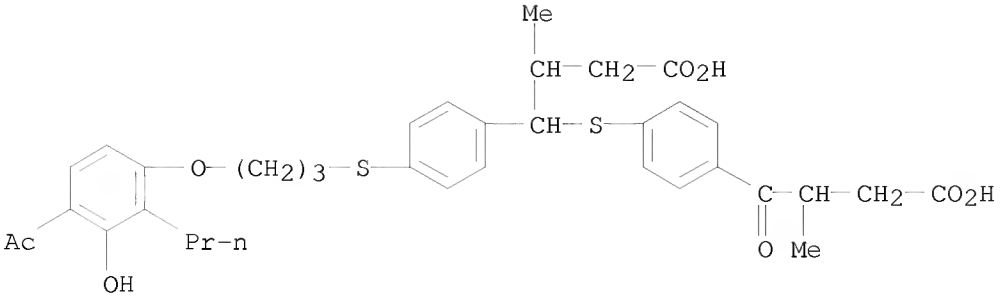
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 6 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 120571-33-7 REGISTRY
ED Entered STN: 12 May 1989
CN Benzenepropanoic acid, α-diazo-β-oxo-2-[(phenylmethyl)sulfinyl]-, ethyl ester (CA INDEX NAME)
MF C18 H16 N2 O4 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

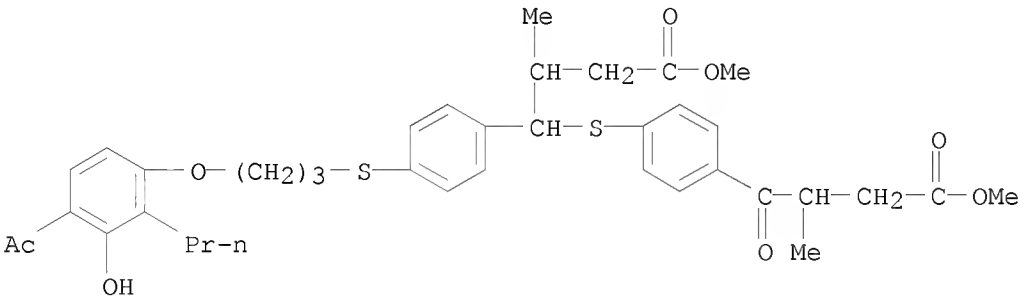
L4 ANSWER 7 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 109010-56-2 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-2-methyl-1-oxopropyl)phenyl]thio]-β-methyl-, [βR*,γR*(S*)]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-2-methyl-1-oxopropyl)phenyl]thio]-β-methyl-, [βR*,γR*(S*)]-(±)-
MF C36 H42 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 8 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-44-7 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(4-methoxy-2-methyl-1,4-dioxobutyl)phenyl]thio]-β-methyl-, methyl ester (CA INDEX NAME)
MF C38 H46 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

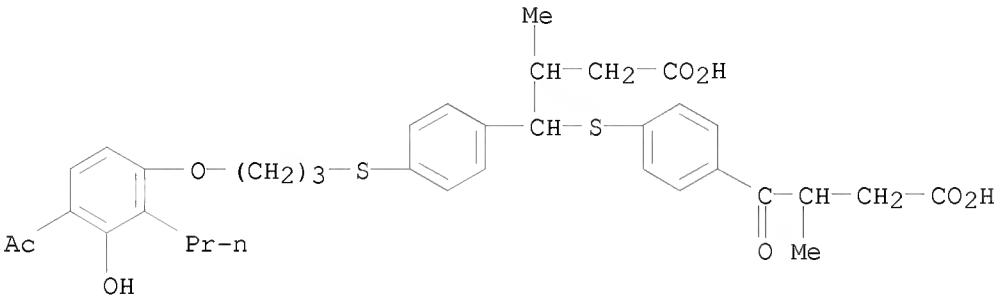


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 9 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-43-6 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-2-methyl-1-

oxopropyl)phenyl]thio]-β-methyl-, [βR*,γR*(R*)]- (9CI)
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-2-methyl-1-oxopropyl)phenyl]thio]-β-methyl-, [βR*,γR*(R*)]-(±)-
MF C36 H42 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

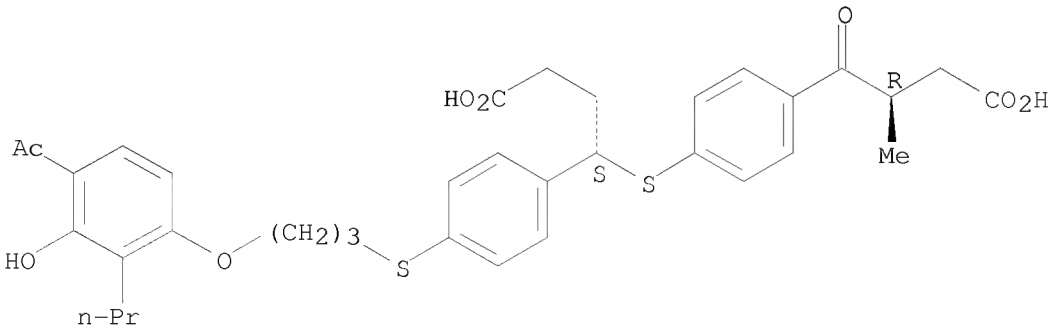


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 10 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-17-4 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[1-[4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]phenyl]-3-carboxypropyl]thio]-β-methyl-γ-oxo-, (R*,S*)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H40 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Relative stereochemistry.

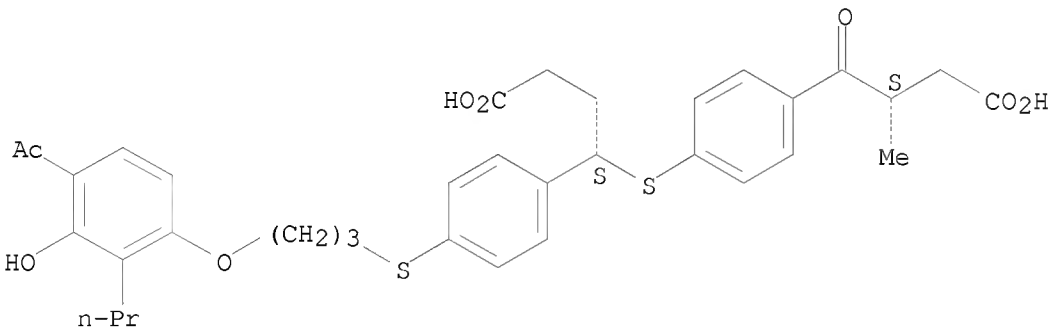


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 11 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-16-3 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[1-[4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]phenyl]-3-carboxypropyl]thio]-β-methyl-γ-oxo-, (R*,R*)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C35 H40 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

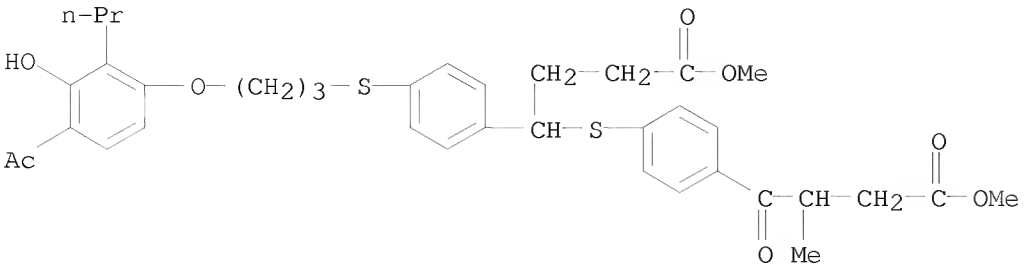
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

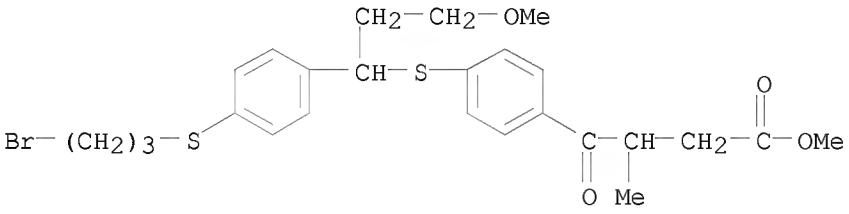
L4 ANSWER 12 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-15-2 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[1-[4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]phenyl]-4-methoxy-4-oxobutyl]thio]-β-methyl-γ-oxo-, methyl ester (CA INDEX NAME)
MF C37 H44 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

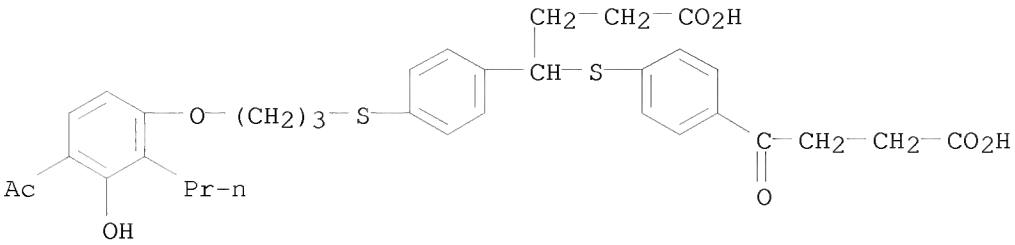
L4 ANSWER 13 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-13-0 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[1-[4-[(3-bromopropyl)thio]phenyl]-3-methoxypropyl]thio]-β-methyl-γ-oxo-, methyl ester (CA INDEX NAME)
MF C25 H31 Br O4 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

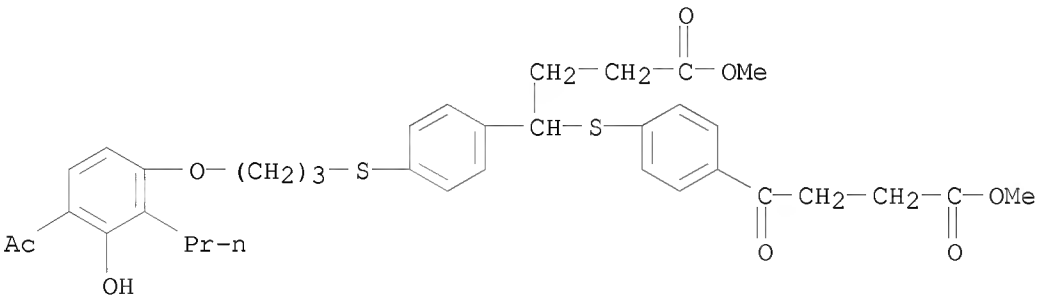
L4 ANSWER 14 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-10-7 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-1-oxopropyl)phenyl]thio]- (CA INDEX NAME)
MF C34 H38 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 15 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-09-4 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(4-methoxy-1,4-dioxobutyl)phenyl]thio]-, methyl ester (CA INDEX NAME)
MF C36 H42 O8 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

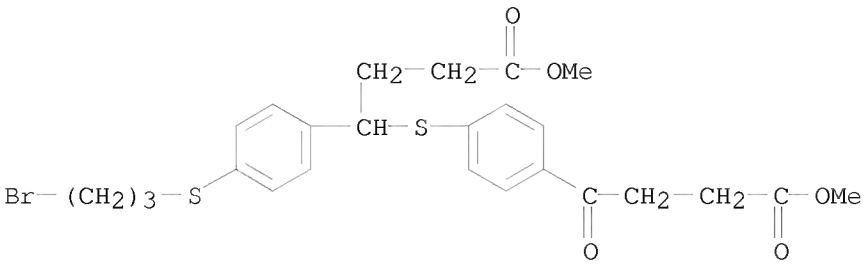


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 16 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 108960-08-3 REGISTRY
ED Entered STN: 03 Jul 1987
CN Benzenebutanoic acid, 4-[(3-bromopropyl)thio]-γ-[[4-(4-methoxy-1,4-dioxobutyl)phenyl]thio]-, methyl ester (CA INDEX NAME)
MF C25 H29 Br O5 S2
SR CA

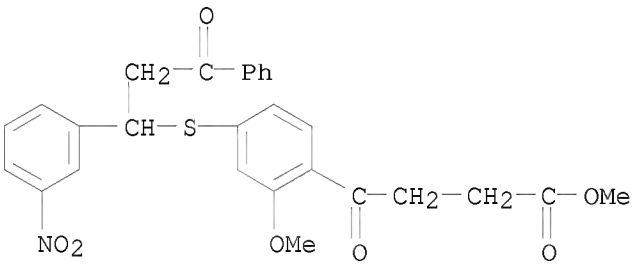
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

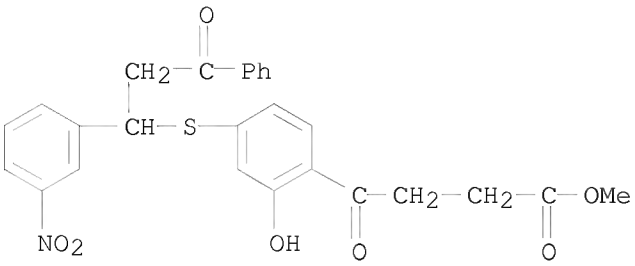
L4 ANSWER 17 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 91540-86-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenebutanoic acid, 2-methoxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo-, methyl ester (CA INDEX NAME)
MF C27 H25 N O7 S
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

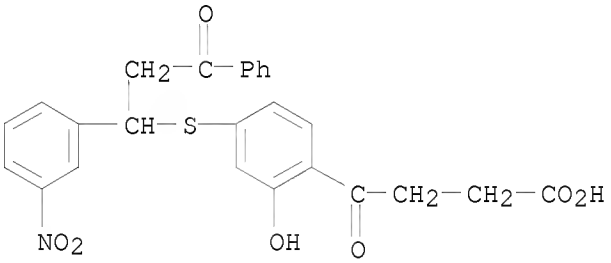
L4 ANSWER 18 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 91540-78-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenebutanoic acid, 2-hydroxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo-, methyl ester (CA INDEX NAME)
MF C26 H23 N O7 S
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 19 OF 19 REGISTRY COPYRIGHT 2009 ACS on STN
RN 91540-77-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenebutanoic acid, 2-hydroxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo- (CA INDEX NAME)
MF C25 H21 N O7 S
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> => s l3
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

```
SAMPLE SEARCH INITIATED 12:12:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     2651 TO ITERATE

 75.4% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        49932 TO    56108
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L3



L6           0 L5

=> dis his

     (FILE 'HOME' ENTERED AT 12:05:27 ON 11 MAR 2009)

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L5            0 S L3

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=> s l4
L7           9 L4

=> d 1-9 bib abs hitstr

L7   ANSWER 1 OF 9  CAPLUS  COPYRIGHT 2009 ACS on STN
AN   2005:177884  CAPLUS <<LOGINID::20090311>>
DN   142:279944
TI   Preparation of phenyl thioethers for the treatment of metabolic disorders
IN   Sharma, Shalini; Von Borstel, Reid W.; Hodge, Kirvin L.
PA   Wellstat Therapeutics Corporation, USA
SO   PCT Int. Appl., 42 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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PI   WO 2005018628        A1    20050303    WO 2004-US26561        20040816
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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU	2004266673	A1	20050303	AU 2004-266673	20040816
CA	2533890	A1	20050303	CA 2004-2533890	20040816
EP	1656127	A1	20060517	EP 2004-781277	20040816
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN	1835743	A	20060920	CN 2004-80023552	20040816
BR	2004013758	A	20061031	BR 2004-13758	20040816
JP	2007502824	T	20070215	JP 2006-523964	20040816
IN	2006DN00452	A	20070831	IN 2006-DN452	20060125
NO	2006000502	A	20060503	NO 2006-502	20060131
KR	2006066730	A	20060616	KR 2006-703221	20060216
MX	2006001963	A	20060531	MX 2006-1963	20060220
US	20070282003	A1	20071206	US 2007-566302	20070301
PRAI US	2003-496533P	P	20030820		
	WO 2004-US26561	W	20040816		

OS CASREACT 142:279944; MARPAT 142:279944

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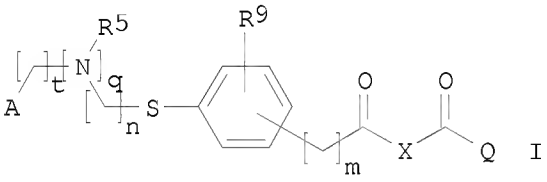

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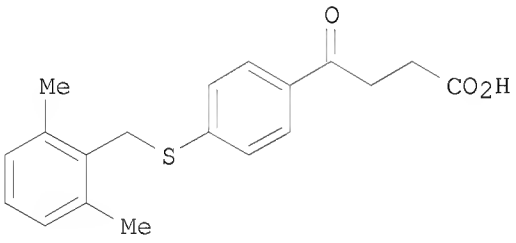


II

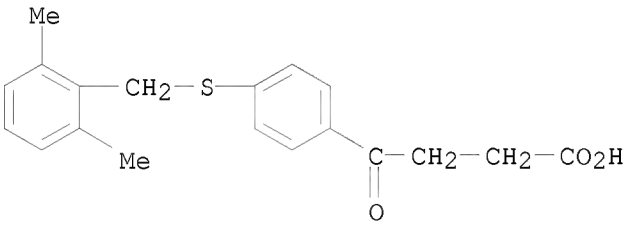
AB The title compds. I [n = 1–2; m, q, t = 0–1; R5 = alkyl; R9 = H, halo, alkyl, alkoxy; A = (un)substituted Ph, cycloalkyl, 5–6 membered heteroarom. ring having 1 or 2 ring heteroatoms selected from N, S and 0 and the heteroarom. ring is covalently bound to the remainder of the

compound I by a ring carbon; X = CH2; Q = OR1 and R1 = Me, Et; or X = CH2CR12R13 or CH2CH(NHAc) (wherein R12, R13 = H, Me), Q = OR1 and R1 = H, alkyl; or X = CH2CH2 and Q = NR10R11 (wherein one of R10 and R11 = H, alkyl or OH, and the other = H); alternatively, when R1 = H, the biol. active agent can be a pharmaceutically acceptable salt of the compound I], useful for the treatment of various metabolic disorders, such as insulin resistance syndrome, diabetes, hyperlipidemia, fatty liver disease, cachexia, obesity, atherosclerosis and arteriosclerosis are disclosed. E.g., a multi-step synthesis of II, starting from 2,6-dimethylbenzyl alc., was given. The pharmaceutical composition comprising the compound I is also disclosed.

IT 847142-00-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of Ph thioethers for the treatment of metabolic disorders)

RN 847142-00-1 CAPLUS

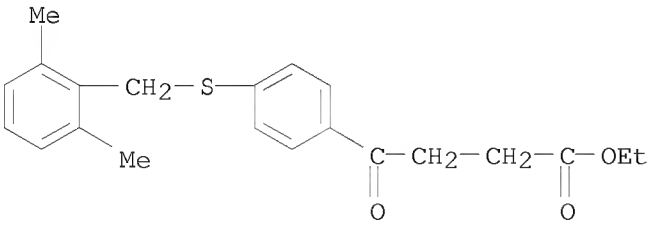
CN Benzenebutanoic acid, 4-[[(2,6-dimethylphenyl)methyl]thio]-γ-oxo- (CA INDEX NAME)



IT 847142-02-3P, Ethyl 4-[4-[(2,6-dimethylbenzyl)thio]phenyl]-4-oxobutyrate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Ph thioethers for the treatment of metabolic disorders)

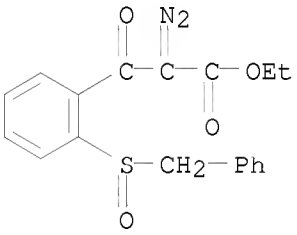
RN 847142-02-3 CAPLUS

CN Benzenebutanoic acid, 4-[[(2,6-dimethylphenyl)methyl]thio]-γ-oxo-, ethyl ester (CA INDEX NAME)



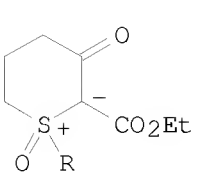
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
AN 2004:624073 CAPLUS <<LOGINID::20090311>>
DN 142:297573
TI Product class 1: sulfur ylides
AU Aggarwal, V.; Richardson, J.
CS Germany
SO Science of Synthesis (2004), 27, 21-104
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review. Preparation and use of sulfur ylides in organic reactions are examined
IT 120571-33-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and use of sulfur ylides in organic reactions)
RN 120571-33-7 CAPLUS
CN Benzenepropanoic acid, α-diazo-β-oxo-2-[(phenylmethyl)sulfinyl]-, ethyl ester (CA INDEX NAME)



RE.CNT 292 THERE ARE 292 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1991:42486 CAPLUS <<LOGINID::20090311>>
DN 114:42486
OREF 114:7393a,7396a
TI Rhodium carbenoid mediated cyclizations. Part 6. Synthesis of cyclic sulfoxonium ylides
AU Moody, Christopher J.; Taylor, Roger J.
CS Dep. Chem., Imp. Coll. Sci., Technol. Med., London, SW7 2AY, UK
SO Tetrahedron (1990), 46(18), 6525-44
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 114:42486
GI



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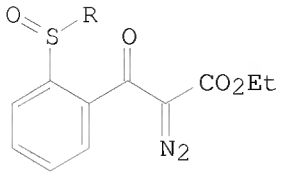

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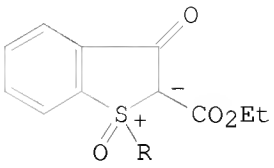


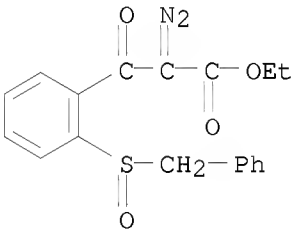
III

AB Rh2(OAc)4-catalyzed cyclization of RS(O)(CH2)3COC(:N2)CO2Et (R = Et, PhCH2, allyl, PhCH:CHCH2) gave 54-84% cyclic sulfoxonium ylides I. In contrast, Rh2(OAc)4-catalyzed decomposition of RS(O)(CH2)4COC(:N2)CO2R1 (R = PhCH:CHCH2, R1 = Et; R = PhCH2, R1 = H) gave complex mixts., with no evidence for the formation of 7-membered ring sulfonium ylides. Heating diazo sulfoxides II (R = Ph, CH2Ph) with Rh2(OAc)4 gave 5-membered sulfoxonium ylides III (R = Ph, CH2Ph) in 70 and 58% yields resp.

IT 120571-33-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rhodium-catalyzed cyclization of)

RN 120571-33-7 CAPLUS

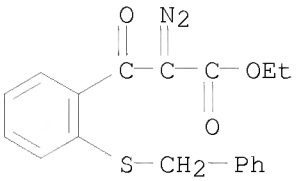
CN Benzenepropanoic acid, α-diazo-β-oxo-2-[(phenylmethyl)sulfinyl]-, ethyl ester (CA INDEX NAME)



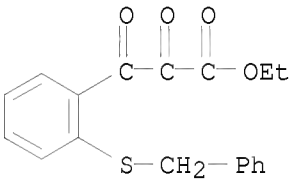
IT 131327-55-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and S-oxidation of, with chloroperbenzoic acid)

RN 131327-55-4 CAPLUS

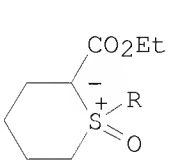
CN Benzenepropanoic acid, α-diazo-β-oxo-2-[(phenylmethyl)thio]-, ethyl ester (CA INDEX NAME)



IT 120571-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 120571-37-1 CAPLUS
CN Benzenepropanoic acid, α,β-dioxo-2-[(phenylmethyl)thio]-, ethyl ester (CA INDEX NAME)



L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1989:212555 CAPLUS <<LOGINID::20090311>>
DN 110:212555
OREF 110:35271a,35274a
TI Rhodium carbenoid-mediated cyclizations. Synthesis and x-ray structures of cyclic sulfoxonium ylides
AU Moody, Christopher J.; Slawin, Alexandra M. Z.; Taylor, Roger J.; Williams, David J.
CS Dep. Chem., Imp. Coll. Sci., Technol. + Med., London, SW7 2AY, UK
SO Tetrahedron Letters (1988), 29(46), 6009-12
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 110:212555
GI



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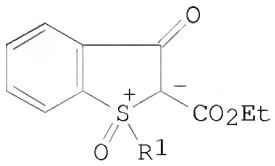


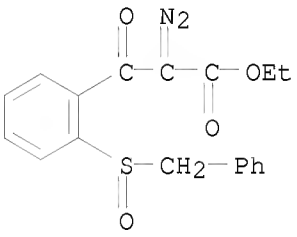
II

AB Rh2(OAc)4-catalyzed decomposition of RS(O)(CH2)3COC(:N2)CO2Et (R = Et, PhCH2, allyl, PhCH:CHCH2) and o-R1S(O)C6H4COC(:N2)CO2Et gives the cyclic sulfoxonium ylides I (same R) and II (same R1), resp. The structures of I (R = allyl) and II (R1 = Ph) were determined by x-ray crystallog.

IT 120571-33-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and intramol. carbenoid cycloaddn. reaction of, rhodium-catalyzed)

RN 120571-33-7 CAPLUS

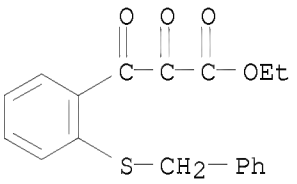
CN Benzenepropanoic acid, α-diazo-β-oxo-2-[(phenylmethyl)sulfinyl]-, ethyl ester (CA INDEX NAME)



IT 120571-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 120571-37-1 CAPLUS

CN Benzenepropanoic acid, α,β-dioxo-2-[(phenylmethyl)thio]-, ethyl ester (CA INDEX NAME)



L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1988:510023 CAPLUS <<LOGINID::20090311>>

DN 109:110023

OREF 109:18318h,18319a

TI Leukotriene antagonists [especially 4-[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propoxy]benzenebutanoic acid derivatives and their sulfur-containing analogs], and their preparation and pharmaceutical formulations

IN Belanger, Patrice C.; Fortin, Rejean; Guindon, Yvan; Rokach, Joshua; Yoakim, Christiane

PA Merck Frosst Canada, Inc., Can.

SO Eur. Pat. Appl., 70 pp.
CODEN: EPXXDW

DT Patent

LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 252639	A1	19880113	EP 1987-305526	19870622
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AU 8774550	A	19871224	AU 1987-74550	19870622
	DK 8703162	A	19880315	DK 1987-3162	19870622
	ZA 8704486	A	19890125	ZA 1987-4486	19870622
	JP 63022537	A	19880130	JP 1987-156413	19870623
	US 5135940	A	19920804	US 1991-672520	19910320
PRAI	US 1986-877655	A	19860623		
	US 1982-422338	B2	19820923		
	US 1983-520052	B2	19830805		
	US 1984-591346	B2	19840319		
	US 1988-253992	B1	19881005		

OS MARPAT 109:110023
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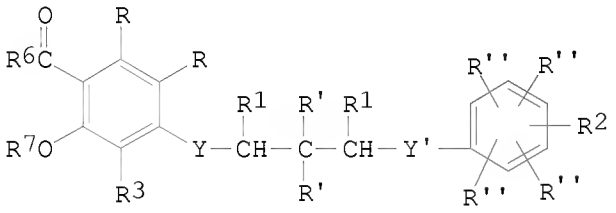

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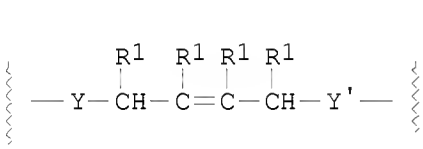

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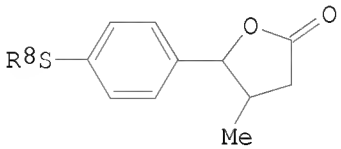

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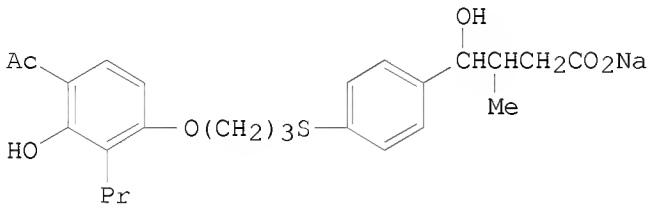


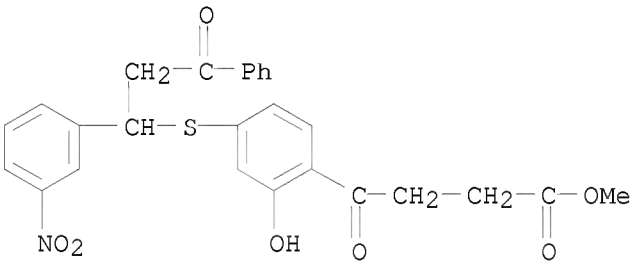
IV

AB The title compds. [I and II; R = H, OH, alkyl, alkenyl, CF3, alkoxy, SH, thioalkyl, Ph, alkylphenyl, halophenyl, PhCH2, phenalkyl, halo, N(R4)2, CO2R4, CH2OR4, CHO, cyano, CF3S, NO2; R' = R4, OR4, CO2R4, N(R4)2, SR4, CH2OR4, CHO; R'R' = O, CH2, OCHR4; R'' = as for R, but excluding OH, SH, and N(R4)2; R1, R4, R7 = H, alkyl; R2 = substituted sidechain with optional unsatn. and terminated by R5; R3 = alkyl, alkenyl; R5 = CO2R4, CH2OH, CHO, tetrazolyl, cyano, etc.; R6 = alkyl, alkoxy, (CH2)rR5 where r = 0-20; Y = O; Y' = O, S, sulfoxide, sulfone, amino, cyanamido] are prepared as leukotriene antagonists. Friedel-Crafts acylation of anisole by

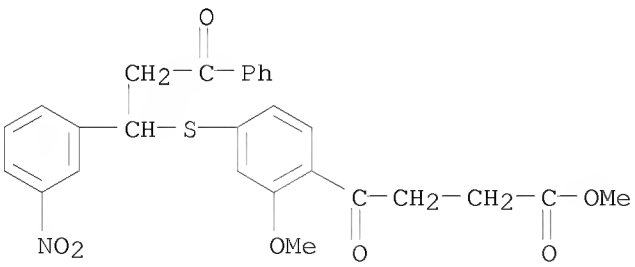
succinic anhydride gave 4-MeOC6H4COCH2CH2CO2H, which was demethylated by HBr/HOAc and esterified by HCl/MeOH to give 4-HOC6H4COCH2CH2CO2Me. Acylation by Me2NC(S)Cl and thermal rearrangement of the dimethylthiocarbamoyl derivative gave 4-[Me2NC(O)S]C6H4COCH2CH2CO2Me, which was methylated by KH/MeI, reduced by NaBH4 in the presence of CsCl, and lactonized by CF3CO2H to give the γ-hydroxy-β-methylbenzenebutanoic acid γ-lactones cis- and trans-III [R8 = 3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]. Saponification gave the crude hydroxyacid, which was treated with CH2N2 to give the Me ester and then coupled with d-α-methoxymandelic acid using DCC. Chromatog. of the diastereomeric methoxymandelates and sep. saponification with NaOH gave the (+)- and (-)-isomers of (phenoxypropylthio)hydroxymethyl benzenebutanoate (βS,γR)-IV (V). (+)- And (-)-V had resp. ED50 values of 1 and 0.21 mg/kg (i.v., 15 min pretreatment) for inhibition of LTD4-induced bronchoconstriction in anesthetized guinea pigs. Capsules may contain I or II 25.0, powdered lactose 573.5, and Mg stearate 1.5 mg/capsule.

IT 91540-78-2P 91540-86-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, as intermediate for leukotriene antagonists)

RN 91540-78-2 CAPLUS
CN Benzenebutanoic acid, 2-hydroxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo-, methyl ester (CA INDEX NAME)



RN 91540-86-2 CAPLUS
CN Benzenebutanoic acid, 2-methoxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo-, methyl ester (CA INDEX NAME)



L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1987:458842 CAPLUS <<LOGINID::20090311>>
DN 107:58842
OREF 107:9769a,9772a
TI Leukotriene antagonists
IN Young, Robert N.; Frenette, Richard; Gauthier, Jacques Yves
PA Merck Frosst Canada, Inc., Can.
SO Eur. Pat. Appl., 87 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 206741	A2	19861230	EP 1986-304665	19860617
	EP 206741	A3	19871223		
	EP 206741	B1	19910410		
	R: AT, BE, CH, DE, FR, GB, LI, LU, NL, SE				
	US 4990526	A	19910205	US 1986-872309	19860609
	CA 1309557	C	19921027	CA 1986-511571	19860613
	DK 8602828	A	19870213	DK 1986-2828	19860617
	AT 62481	T	19910415	AT 1986-304665	19860617
	JP 62059239	A	19870314	JP 1986-142459	19860618
PRAI	US 1985-746203	A	19850618		
	EP 1986-304665	A	19860617		

OS MARPAT 107:58842
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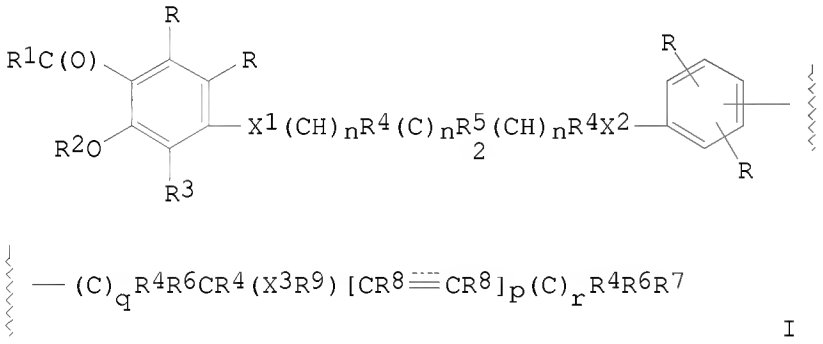


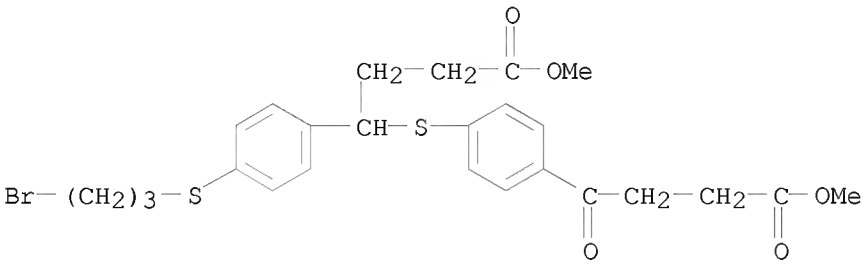
I

AB Title compds. I (R = H, HO, alkyl, alkenyl, (un)substituted Ph, halo, F3C, PhCH2, etc.; R1 = H, alkoxy, alkyl; R2 = H, alkyl, R4CO, R4OCH2, R4 = H, alkyl; R3 = alkyl, alkenyl; R5 = H, OR2, alkyl, etc.; R6 = H, HO, alkyl; R7 = CO2R4, CHO, CH2OH, tetrazolyl, etc.; R8 = H, alkyl, absent if triple bond present; R9 = R3, alkylheterocyclyl, etc.; n = 0-6; p = 0-2; q = r = 0-4; X1, X2, X3 = O, S, SO, SO2, NCN, etc.) and their salts, were prepared I are antagonists of slow reacting substance of anaphylaxis and the leukotrienes C4, D4 and E4, and thus are inhibitors of the symptoms induced by leukotrienes in humans (no data). Thus, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-β-methyl-γ-hydroxybenzenebutanoic acid γ-lactone was converted to the

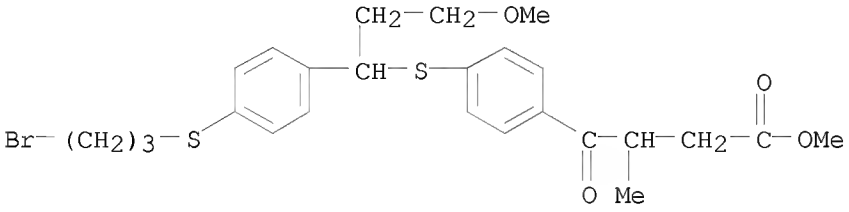
Me ester of the cleaved lactone, which in ClCH2CH2Cl was treated with Me 7-mercapto-4-oxo-4H-1-benzopyran-2-carboxylate in presence of ZnI2, followed by hydrolysis to give di-Na αR, βR and αR, βS-7-[[α-[4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]phenyl]-γ-carboxy-β-methylpropyl]thio]-4-oxo-4H-1-benzopyran-2-carboxylate. Pharmaceutical formulations containing I are given.

IT 108960-08-3P 108960-13-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with acetophenone derivative)

RN 108960-08-3 CAPLUS
CN Benzenebutanoic acid, 4-[(3-bromopropyl)thio]-γ-[[4-(4-methoxy-1,4-dioxobutyl)phenyl]thio]-, methyl ester (CA INDEX NAME)

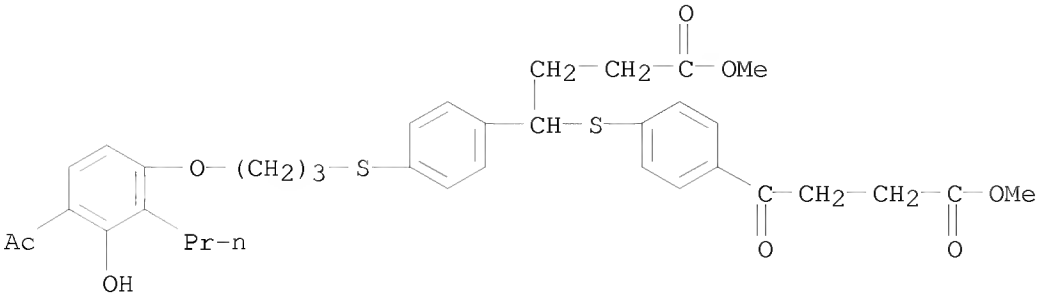


RN 108960-13-0 CAPLUS
CN Benzenebutanoic acid, 4-[[1-[4-[(3-bromopropyl)thio]phenyl]-3-methoxypropyl]thio]-β-methyl-γ-oxo-, methyl ester (CA INDEX NAME)

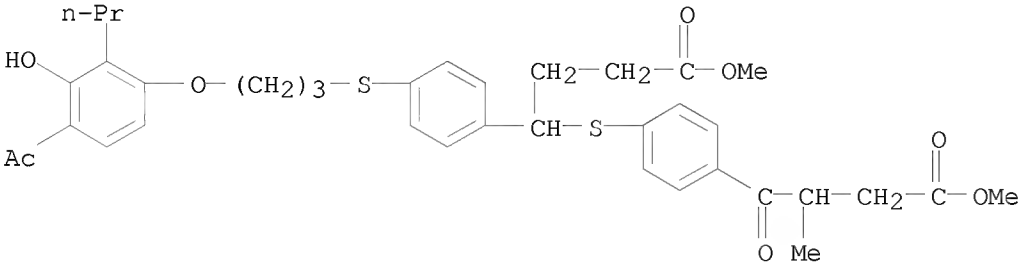


IT 108960-09-4P 108960-15-2P 108960-44-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)

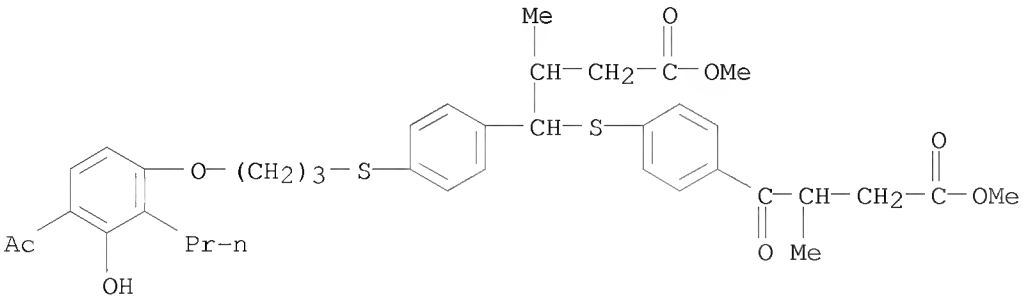
RN 108960-09-4 CAPLUS
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(4-methoxy-1,4-dioxobutyl)phenyl]thio]-, methyl ester (CA INDEX NAME)



RN 108960-15-2 CAPLUS
CN Benzenebutanoic acid, 4-[[1-[4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]phenyl]-4-methoxy-4-oxobutyl]thio]-β-methyl-γ-oxo-, methyl ester (CA INDEX NAME)



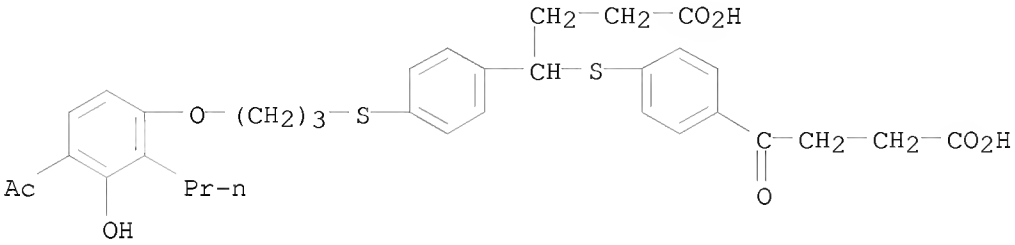
RN 108960-44-7 CAPLUS
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(4-methoxy-2-methyl-1,4-dioxobutyl)phenyl]thio]-β-methyl-, methyl ester (CA INDEX NAME)



IT 108960-10-7P 108960-16-3P 108960-17-4P
108960-43-6P 109010-56-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

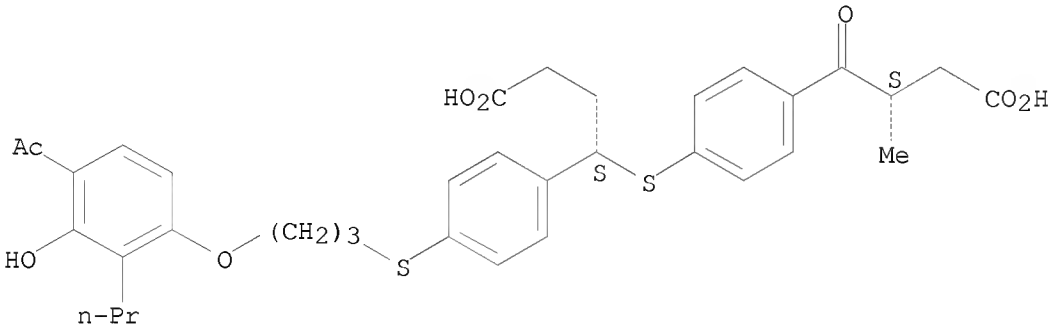
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as leukotriene antagonist)

RN 108960-10-7 CAPLUS
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-1-oxopropyl)phenyl]thio]- (CA INDEX NAME)



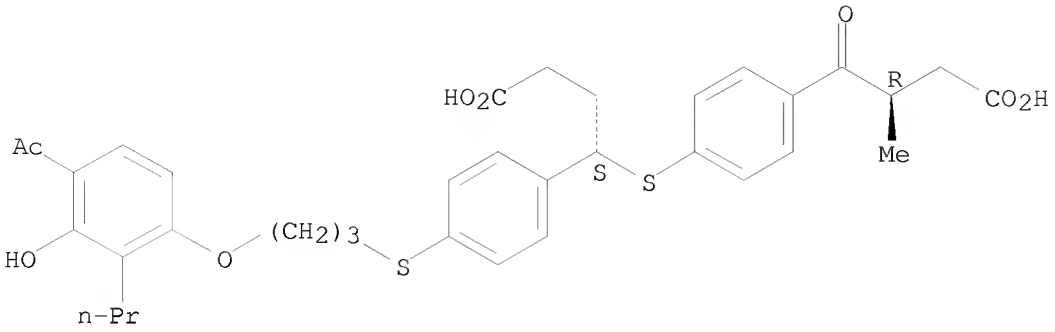
RN 108960-16-3 CAPLUS
CN Benzenebutanoic acid, 4-[[1-[4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]phenyl]-3-carboxypropyl]thio]-β-methyl-γ-oxo-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

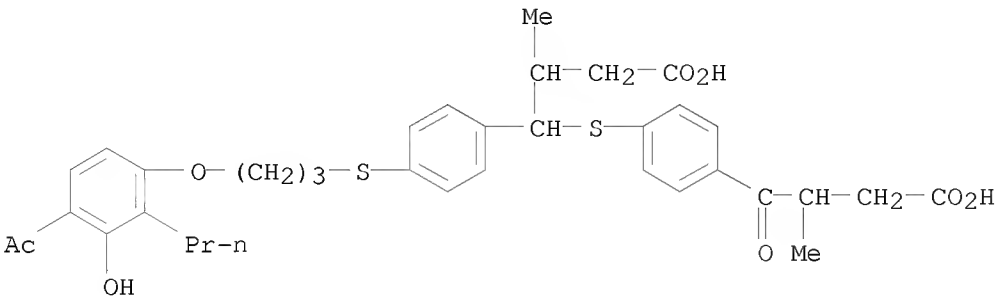


RN 108960-17-4 CAPLUS
CN Benzenebutanoic acid, 4-[[1-[4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]phenyl]-3-carboxypropyl]thio]-β-methyl-γ-oxo-, (R*,S*)- (9CI) (CA INDEX NAME)

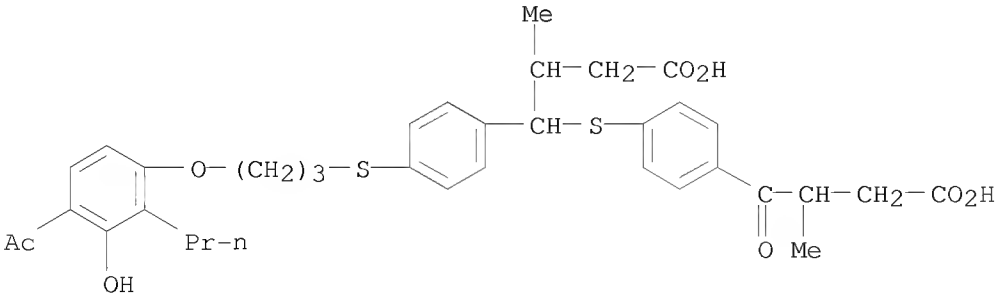
Relative stereochemistry.



RN 108960-43-6 CAPLUS
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-2-methyl-1-oxopropyl)phenyl]thio]-β-methyl-, [βR*,γR*(R*)]- (9CI) (CA INDEX NAME)



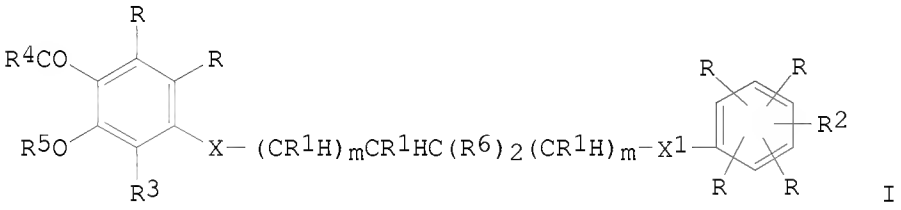
RN 109010-56-2 CAPLUS
CN Benzenebutanoic acid, 4-[[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propyl]thio]-γ-[[4-(3-carboxy-2-methyl-1-oxopropyl)phenyl]thio]-β-methyl-, [βR*,γR*(S*)]- (9CI) (CA INDEX NAME)



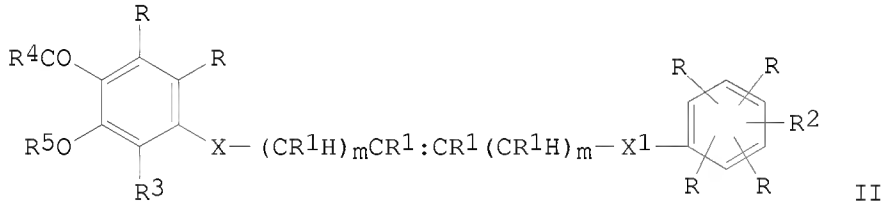
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1986:109232 CAPLUS <<LOGINID::20090311>>
DN 104:109232
OREF 104:17293a
TI Use of leukotriene antagonists for producing cytoprotective pharmaceutical compositions and process for producing cytoprotective pharmaceutical compositions
IN Goldenberg, Marvin M.
PA Merck and Co., Inc. , USA
SO Eur. Pat. Appl., 115 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 156233	A2	19851002	EP 1985-102787	19850312
	EP 156233	A3	19860219		
	R: CH, DE, FR, GB, IT, LI, NL				
	JP 60209519	A	19851022	JP 1985-53506	19850319
PRAI	US 1984-590815	A	19840319		
	US 1984-685102	A	19841221		

OS MARPAT 104:109232
GI



I



II

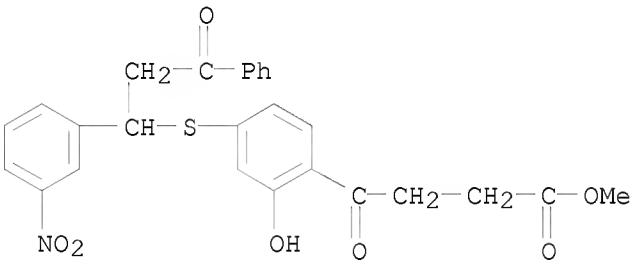
AB The title compds. I and II (R = H, OH, C1-6 alkyl or alkoxy, C2-6 alkenyl, CF3, SH, cyano, NO2, (un)substituted Ph, etc.; R1 = H, C1-3 alkyl; R2 = (un)substituted alkanoyl, etc.; R3 = C1-6 alkyl, C3-6 alkenyl; R4 = C1-6 alkyl or alkoxy, etc., R5 = C1-6 alkyl, R6CO, R6OCH2, R6 = H, C1-6 alkyl, CO2R6, CH2OR6, cyano, NO2, or F3CS, etc.; R6R6 = O, CH2, epoxy; X = O, S, S(O); X1 = X, CH2, CO; m = 0-6) and their salts useful as leukotriene antagonist pharmaceuticals inducing cytoprotection were prepared Thus, 4-mercaptobenzene-γ-oxobutyronitrile (prepared in 4 steps from

4-methylthiobenzaldehyde), 4-(3-bromopropoxy)-2-hydroxy-3-propylacetophenone, and K2CO3 were dissolved in MeCOEt and refluxed to give 4-[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propythio]benzene-γ-oxobutyronitrile, which at 30 mg/kg orally to rats showed 89.4% inhibition of indomethacin-induced ulcer. A capsule (600 mg) formulation contained I or II 0.07-70, lactose 248.5-598.3 and Mg stearate 1-1.5 g.

IT 91540-78-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)

RN 91540-78-2 CAPLUS

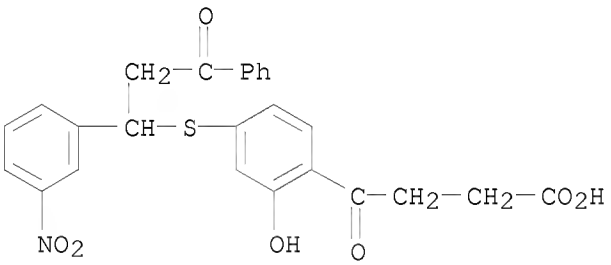
CN Benzenebutanoic acid, 2-hydroxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo-, methyl ester (CA INDEX NAME)



IT 91540-77-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and esterification-deprotection of)

RN 91540-77-1 CAPLUS

CN Benzenebutanoic acid, 2-hydroxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo- (CA INDEX NAME)



L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1984:510548 CAPLUS <<LOGINID::20090311>>

DN 101:110548

OREF 101:16868h,16869a

TI Leukotriene antagonists and compositions containing them

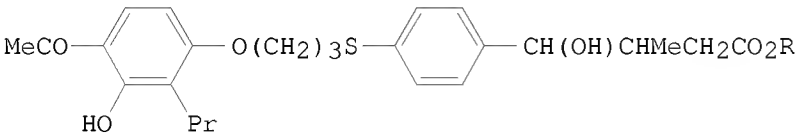
IN Belanger, Patrice C.; Fortin, Rejean; Guindon, Yvan; Rokach, Joshua; Yoakim, Christiane

PA Merck Frosst Canada, Inc., Can.

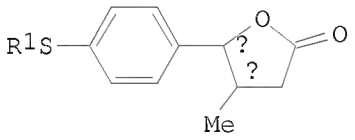
SO Eur. Pat. Appl., 120 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 104885	A1	19840404	EP 1983-305588	19830921
	EP 104885	B1	19860604		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	IL 69691	A	19880131	IL 1983-69691	19830912
	AU 8319190	A	19840329	AU 1983-19190	19830916
	AU 557953	B2	19870115		
	AT 20233	T	19860615	AT 1983-305588	19830921
	CA 1210770	A1	19860902	CA 1983-437216	19830921
	DK 8304327	A	19840504	DK 1983-4327	19830922
	ZA 8307048	A	19850529	ZA 1983-7048	19830922
	JP 59139342	A	19840810	JP 1983-175237	19830924
	US 5135940	A	19920804	US 1991-672520	19910320
PRAI	US 1982-422338	A	19820923		
	US 1983-520052	B2	19830805		
	EP 1983-305588	A	19830921		
	US 1984-591346	B2	19840319		
	US 1986-877655	B1	19860623		
	US 1988-253992	B1	19881005		

GI



I

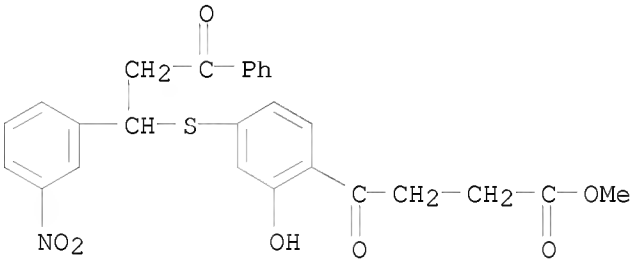


II

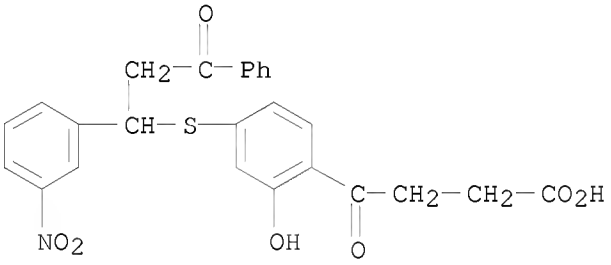
AB Benzenebutanoic acid derivs. (146 compds.), including I (R = Na), were prepared Thus, PhOMe was acylated by succinic anhydride to give 4-MeOC6H4CO(CH2)2CO2H which was demethylated and esterified to give 4-HOC6H4CO(CH2)2CO2Me. The latter compound was esterified with Me2NCSCl, thermally rearranged, and methylated to give 4-[Me2NC(O)S]C6H4COCHMeCH2CO2Me. This ester was hydrolyzed, reduced, and cyclized to give lactones βS*,γR*-II and βR*,γR*-II (R1 = Me2NCO). βS*,γR*-II was saponified and alkylated with 4'-(3-bromopropoxy)-3'-propyl-2'-hydroxyacetophenone to give βS*,γR*-II [R1 = 4,3,2-MeCO(HO)(Pr)C6H2O(CH2)3] which was hydrolyzed to βS*,γR*-I (R = H). The latter compound was

resolved to give (+)- and (-)-βS*,γR*-I (R = Na). The ED50 for these compds. to inhibit leukotriene D4-induced bronchoconstriction in guinea pigs were 1 and 0.21 mg/kg (i.v.), resp.

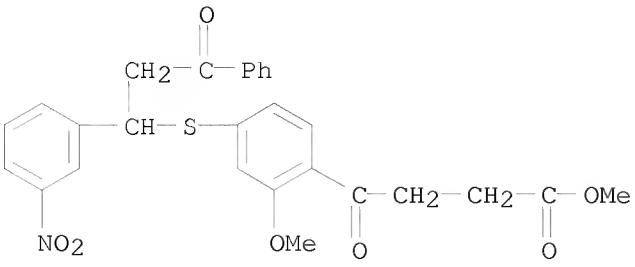
IT 91540-78-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dealkylation of)
RN 91540-78-2 CAPLUS
CN Benzenebutanoic acid, 2-hydroxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo-, methyl ester (CA INDEX NAME)



IT 91540-77-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification and methylation of)
RN 91540-77-1 CAPLUS
CN Benzenebutanoic acid, 2-hydroxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo- (CA INDEX NAME)



IT 91540-86-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 91540-86-2 CAPLUS
CN Benzenebutanoic acid, 2-methoxy-4-[[1-(3-nitrophenyl)-3-oxo-3-phenylpropyl]thio]-γ-oxo-, methyl ester (CA INDEX NAME)



L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1955:53500 CAPLUS <<LOGINID::20090311>>
DN 49:53500
OREF 49:10267g-i,10268a-d
TI Derivatives of 5-o-mercaptophenyl-3-methyl-1-phenylpyrazole
AU Barry, W. J.; Finar, I. L.
CS Northern Polytech., London
SO Journal of the Chemical Society (1954) 138-40
CODEN: JCSOA9; ISSN: 0368-1769
DT Journal
LA Unavailable
AB Some new (oo-substituted-phenyl)pyrazoles are prepared in which ring-closure is effected between substituent groups to form a new polycyclic system. o-PhCH2SC6H4CO2H heated 0.5 hr. with 2-3 moles SOCl2 gives 60% of the acid chloride (I), m. 121-2°. I (1.1 moles) and 1 mole AcCH2CO2Et in NaOEt yields 27% PhCH2SC6H4CO2Et (II), m. 68°, alone or mixed with II prepared by heating an excess of I with EtOH. Acidification of the filtrate gives 73% of the diketo ester (III); Cu derivative, bluish-green crystals from CHCl3-ligroine. III (1 mole) heated 2 hrs. at 100° with 1.1 moles PhNHNH2 in HOAc affords 83% Et ester (IV), m. 121-2°, of 5-o-mercaptophenyl-3-methyl-1-phenyl-4-pyrazolecarboxylic acid (V), m. 236° (decomposition). V heated at 250-5° for 1-1.5 hrs. decarboxylates to yield 60% 5-o-benzylthiophenyl-3-methyl-1-phenylpyrazole (VI), m. 110°. Cl passed 0.5 hr. through 40 g. IV, in 1 l. HOAc and 25 ml. H2O at 0° and the solution set aside 10 min. gives 36 g.Et5-o-chlorosulfonylphenyl-3-methyl-1-phenyl-4-pyrazolecarboxylate (VII), m. 155-6°; anilide, m. 157.5°. Similar chlorination of either V or VI gives 80% yield 4-chloro-5-o-chlorosulfonylphenyl-3-methyl-1-phenylpyrazole (VIII), m. 145°. VII (12 g.) kept 12 hrs. at room temperature with 10 g. Zn dust, 100 ml. HOAc, and 20 ml. concentrated HCl, 20 ml. more HCl added, the solution left 1 hr. longer, then treated with H2O to turbidity, gave next morning 9.5 g. Et 3-methyl-1-phenyl-5-o-sulfinophenyl-4-pyrazolecarboxylate (IX), m. 186° (sealed tube), hydrolyzed with 10% KOH-EtOH in 0.5 hr. to 82% of the corresponding carboxylic acid (X), m. 244° (sealed tube). IX (10 g.) refluxed in 100 ml. HOAc and 100 ml. 3N H2SO4 and treated portionwise with 25 g. Zn dust during 1.5 hrs. gives 2-3 g. 5-o-mercaptophenyl-3-methyl-1-phenyl-4-pyrazolecarboxylic acid lactone (XI), m. 208-10°, also prepared by the addition of concentrated HCl to a refluxing solution of IX in HOAc with granulated Zn. XI refluxed several min. with 20% KOH-EtOH and acidified gives the

thiol (XII), m. 158-60°, frothing and resolidifying to m. again at 208-10°, which forms white and yellow ppts. with HgCl2 and Pb(OAc)2, resp. The addition of concentrated HCl to XII in refluxing EtOH gives XI. XII warmed with 10% Na2CO3 solution and PhCH2Cl forms 5-o-benzylthiophenyl-3-methyl-1-phenyl-4-pyrazolecarboxylic acid (XIII), m. 235-6°. The Et ester of XIII (7.5 g.) heated 15 min. with 100 ml. 10% KOH-EtOH gives 5.2 g. free acid, which, heated 1.5 hrs. at 250-70°, yields 5-o-benzylsulfonylphenyl-3-methyl-1-phenylpyrazole (XIV), m. 182-3°. VI (0.75 g.) in 10 ml. HOAc heated 1 hr. at 100° with 3 ml. 30% H2O2 yields 0.5 g. XIV. XIV (1 g.) heated 35 hrs. with 25 g. 5% Na-Hg in 25 ml. EtOH gives o(3-methyl-1-phenyl-5-pyrazolyl)benzenesulfinic acid (XV), characterized by conversion with BzCl in excess K2CO1, to the sulfone (XVI), m. 180-2°. The Et ester of XIII (1 g.) refluxed 9 hrs. with 10 g. Raney Ni in 50 ml. EtOH gives Et 1,5-diphenyl-4-pyrazolecarboxylate (XVII), m. 119-21°. The identity of XVII is confirmed by hydrolysis to the acid, m. 205°.

IT 857559-32-1P, Acetoacetic acid, 2-[o-(benzylthio)benzoyl]-, ethyl ester, Cu derivative
RL: PREP (Preparation)
(preparation of)

RN 857559-32-1 CAPLUS

CN Benzenepropanoic acid, α-acetyl-β-oxo-2-[(phenylmethyl)thio]-, ethyl ester (CA INDEX NAME)